

Icosadeltahedral geometry of fullerenes, viruses and geodesic domes

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I discuss the symmetry of fullerenes, viruses and geodesic domes within a unified framework of icosadeltahedral representation of these objects. The icosadeltahedral symmetry is explained in details by examination of all of these structures. Using Euler's theorem on polyhedra, it is shown how to calculate the number of vertices, edges, and faces in domes, and number of atoms, bonds and pentagonal and hexagonal rings in fullerenes. Caspar-Klug classification of viruses is elaborated as a specific case of icosadeltahedral geometry.

I. INTRODUCTION

Although the fullerene molecules were previously predicted and discussed¹, it was quite a surprise for largest part of the scientific community when Kroto *et al* published a paper announcing their experimental discovery². Some part of this surprise can surely be attributed to amazingly symmetrical arrangement of carbon atoms in the most abundant of all the fullerene molecules - Buckminsterfullerene or C₆₀. Kroto and colleagues named this molecule after Richard Buckminster Fuller who was an American designer, inventor and architect² most recognized for popularizing geodesic domes - networks of interconnected struts forming a (hemi)spherical grid. Fuller constructed domes as an alternative to architecture that was dominant in 1960's in USA. Most famous of them was used to house American pavilion for the World Expo exhibition in Montreal in year 1967. Geodesic domes that Fuller constructed were not chiral³, i.e. their mirror image retained their symmetry. Even before the discovery of fullerenes it became clear that achiral domes that Fuller constructed belong to a larger class of mathematical structures called icosadeltahedra. Extending Fuller's design ideas⁴, in year 1962 Donald Caspar and Aaron Klug constructed the first theory that explained the features of most of the so-called "spherical" (icosahedral) viruses known at the time⁵.

It is intriguing that objects so different in size (fullerenes 1 nm, viruses 100 nm, and geodesic domes 100 m) share the same design and symmetry. The reason for this is that all these objects are built up of nearly identical elements (carbon atoms in fullerenes, proteins in viruses, and struts in geodesic domes) that have to arrange so to fully enclose the object interior i.e. to form a cage-like structure. The aim of this paper is to explain the design principles and symmetries of a large subset of these structures that has an icosadeltahedral symmetry.

II. ICOSADELTAHEDRAL GEODESIC DOMES

Icosadeltahedral geodesic domes can be mathematically described as triangulations of the spherical surface (or a part of it) with the icosahedral "backbone". A visual representation of this statement is shown in Fig.

1. Icosahedron (shown in the upper left corner of Fig. 1) is a platonic solid consisting of twenty equilateral triangles and twelve vertices. When the spherical surface is covered with triangles so that the icosahedral nature of the triangulation is preserved, the twelve icosahedral vertices become special points. These twelve points become the only ones that have *five* nearest neighboring points - all the other points have *six* nearest neighbors. In Fig. 1 the neighboring points of the icosahedral vertices are outlined as thick pentagons. As Fig. 1 illustrates, there are many ways to triangulate a sphere so that there are twelve points that make the vertices of an icosahedron and have five nearest neighbors, all other points having six nearest neighboring points. All of these triangulations are called *icosadeltahedral*. Deltahedron is a polyhedron whose faces are all equilateral triangles. Strictly speaking the icosadeltahedral geodesic domes are *not* (icosadeltahedra since all of the triangles that they consist of are not equilateral. The requirement that all of the polyhedral faces be equilateral triangles necessarily produces aspherical (spiky) polyhedra. Nevertheless, the icosadeltahedral geodesic domes have the same symmetry as an icosadeltahedron which is a spiky shape shown in Fig. 1. In fact the domes can be considered as projections of icosadeltahedra on their circumscribed spheres. In the following the word dome is used only for icosadeltahedral geodesic dome.

Each of the domes can be characterized by two non-negative integers, denoted by m and n in the following. These can be thought of as numbers of "jumps" through the vertices of a dome that need to be performed in order to reach a center of a pentagon from its neighboring pentagon. Except for $(m, 0)$ dome, the jumps need to be directed along two different spherical geodesics (the shortest lines between two points on a sphere), m along one of them, and n along another one, making an angle of 60 degrees with the first one. To be definite, we need to specify whether the "jumper" needs to turn left or right after the m jumps along the first spherical geodesic. In what follows, I shall assume the left turn and denote the symmetry of icosadeltahedral structures by (m, n) . Were the other convention chosen, the (m, n) dome in our convention would correspond to (n, m) dome in the alternative convention. The domes with $m \neq n; m, n > 0$ are *chiral*. This means that their mirror image has differ-

ent symmetry. A mirror image of (m, n) dome is (n, m) dome. This is illustrated in the upper-right corner of Fig. 1 for $(3, 2)$ dome.

From m and n one can calculate the number of triangles in a dome. The number of triangles per one spherical segment bounded by three spherical geodesic passing through neighboring fivefold coordinated vertices (outlined on a $(4, 4)$ dome in Fig. 1) is

$$T = m^2 + n^2 + mn, \quad (1)$$

so that the total number of triangles (or faces) in an icosadeltahedron is

$$f = 20T. \quad (2)$$

T is called the triangulation number or simply the T-number. It adopts special integer values, $T = 1, 3, 4, 7, 9, 12, 13, \dots$. Instead of m and n integers, the T-number can be used to classify the icosadeltahedral symmetry. The problem with this choice is that it doesn't discriminate between (m, n) and (n, m) domes. That is why the T-number is sometimes used in combination with words *laevo* (left) and *dextro* (right) to resolve this ambiguity. For example, $(2, 1)$ structure in our convention would be in this case denoted as $T = 7_{laevo}$ or $T = 7_l$ or simply $T = 7$, while $(1, 2)$ structure would be denoted as $T = 7_{dextro}$ or $T = 7_d$ ⁷. From the known number of polyhedron faces (f) one can proceed to find the number of its vertices (v) and edges (e) by using Euler's theorem on polyhedra⁶ which relates these nonzero integer quantities as

$$v - e + f = 2. \quad (3)$$

This equation is valid for polyhedra that are homeomorphic to the sphere, i.e. their topology is the same as that of a sphere, which is the case of interest to us. In icosadeltahedral domes twelve vertices belong to five edges - these are located at the vertices of an icosahedron. All the other vertices belong to six edges, i.e. six edges meet at those vertices. Each edge is bounded by two vertices and all these fact together can be used to relate e and v as

$$2e = 5 \cdot 12 + 6 \cdot (v - 12) = 60 + 6(v - 12). \quad (4)$$

In combination with Euler's theorem, one obtains that

$$v = \frac{f}{2} + 2 = 10T + 2, \quad (5)$$

and

$$e = \frac{3f}{2} = 30T. \quad (6)$$

III. ICOSAHEDRAL FULLERENES

Fullerene molecules are carbon cages in which all carbon rings are either pentagonal or hexagonal and all carbon atoms make three covalent bonds with their nearest

neighbors. This type of bonding is also present in the planes of carbon atoms in graphite (graphene planes). It is called sp^2 bonding, in contrast to sp^3 bonding that is characteristic of diamond (in diamond each of the carbon atoms is bonded with *three* nearest neighboring atoms). There are many different structures that can be made of carbon atoms connected with sp^2 bonds, at least conceptually (see e.g. Refs. 8,9). Quite a different question is whether such structures can be experimentally obtained. The icosadeltahedral symmetry of geodesic domes is characteristic of a class of especially symmetric fullerene molecules, sometimes called icosahedral fullerenes, or giant icosahedral fullerenes in case that molecules contain more than about 100 carbon atoms. Buckminsterfullerene belongs to this class (its "companion" molecule C_{70} that was discovered simultaneously² does not, however). The symmetry of these carbon molecules can be obtained from icosadeltahedral domes by placing carbon atoms in (bary)centers of every triangle in the dome. The newly obtained set of points (carbon atoms) is then ordered so that each point is connected with its three nearest neighbors, i.e. the carbon-carbon bonds are established (this procedure is illustrated in the upper-right corner of Fig. 2). This fulfills the basic chemical requirement for carbon atoms in sp^2 bonding electronic configuration. The thus obtained structure contains now twelve pentagonal carbon rings (pentagons) and certain number of hexagonal carbon rings (hexagons), depending on the T-number of the dome. The starting dome and the fullerene-like polyhedron that was obtained from it are called *dual polyhedra*. The (m, n) symmetry that was characteristic of the dome will also be characteristic of its dual fullerene-like polyhedron, but now the "jumping" that characterizes icosadeltahedral symmetry is allowed only through the centers of pentagons and hexagons (not along the carbon-carbon bonds). I have used the term "fullerene-like polyhedron" since the true fullerene molecules will in general be different from the polyhedron obtained by a simple mathematical dualization of the dome. The domes are icosadeltahedral triangulations of the sphere and this necessarily means that the lengths of triangular edges are not all the same. In particular, they are considerably shorter in the neighborhood of icosahedral vertices, and this will pertain also in the dual polyhedra. This feature is also characteristic of Fuller's geodesic constructions². However, the fullerene molecules are more than mathematical entities and their exact shape is determined by energetics of carbon-carbon interactions. Carbon-carbon bonds are much easier to bend than to stretch⁸, so the shape of the fullerene molecule will be such to keep the nearest-neighbor carbon-carbon distances as uniform as possible and as close to their equilibrium value as possible (the equilibrium length of carbon-carbon bonds in infinitely large graphene plane is about 1.42 Å). This means that large enough fullerenes will necessarily be aspherical, looking more like an icosahedron with vertices slightly above the centers of carbon pentagons as the molecules

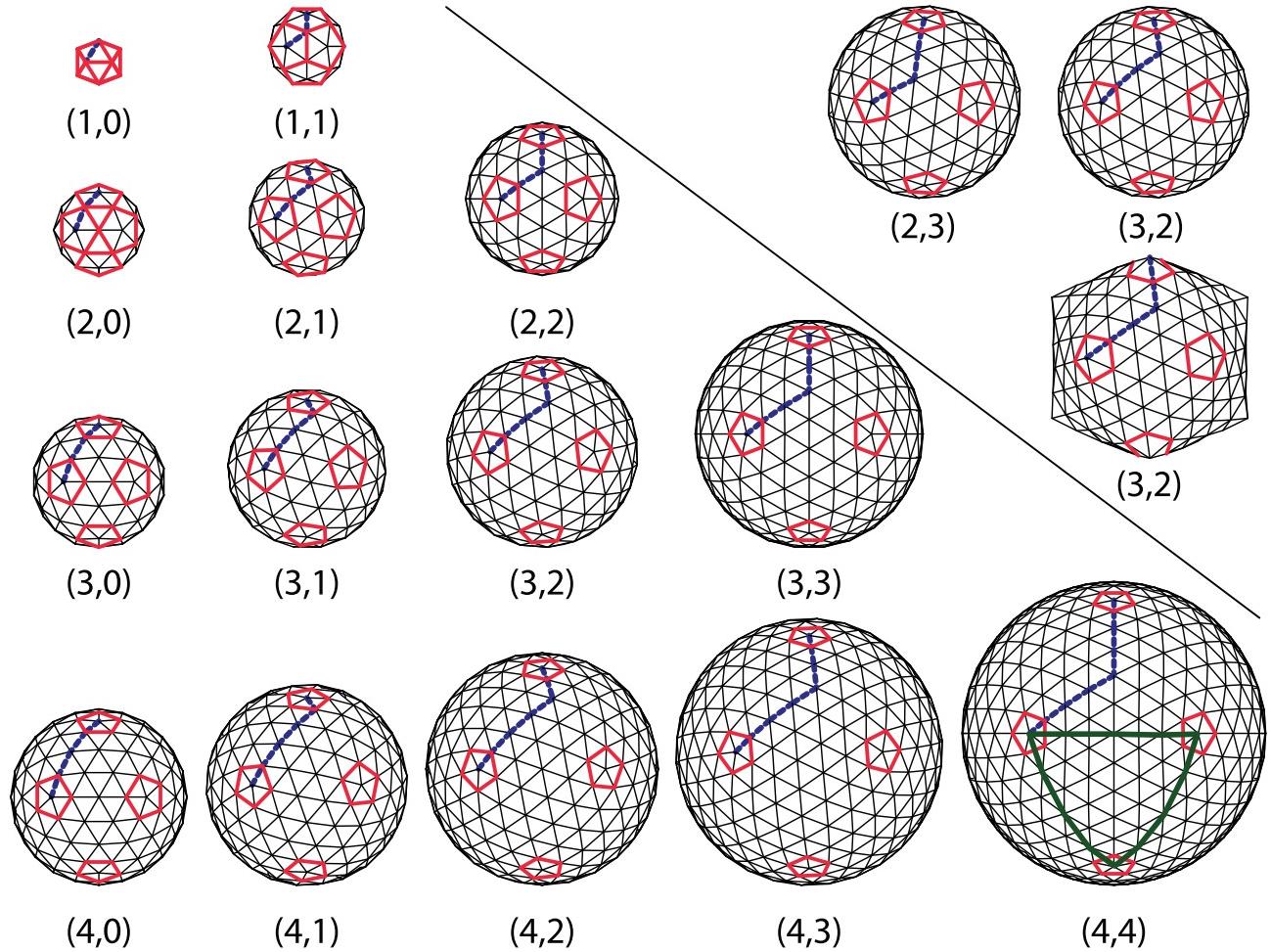


FIG. 1: Gallery of icosadeltahedral geodesic domes for $m > n$ and $m < 5$. For the sake of clarity, the back sides of geodesic domes are not shown, i.e. only half of the dome and four of twelve icosahedral vertices can be seen. The upper-right corner of the figure contains comparison between chiral $(3, 2)$ and $(2, 3)$ domes. Note that they are mirror images. The spiky shape is a $(3, 2)$ icosadeltahedron (all of its faces are equilateral triangles).

get larger¹⁰. Figure 2 displays a gallery of icosahedral fullerenes. Their shape is not merely a mathematical construction obtained by dualization of a dome, but a true minimum of energy, calculated by using the realistic model of energetics of carbon sp^2 bonding¹¹ as described in Ref. 8. Note that the Buckminsterfullerene $(1, 1)$ is perfectly spherical, i.e. all of its carbon atoms are equally distanced from the geometrical center of the molecule. A high degree of sphericity is also present in $(2, 0)$ fullerene, but already in $(2, 1)$ fullerene a clear icosahedral shape of the molecule develops and this becomes more prominent in larger molecules. There is a long standing debate (perhaps of academic value only) concerning the shape of *asymptotic* icosahedral fullerenes, i.e. those that contain extremely large (infinite) number of carbon atoms. Studies based on continuum elasticity of the icosadeltahedral shells^{12,13} and on microscopic models of carbon-carbon bonding¹⁴ predict that the asymptotic shape is a perfect icosahedron.

A way to better comprehend the symmetry of

fullerenes is to "unfold" them so that they become polygonal pieces of graphene. Alternatively, one can also think about this procedure, illustrated in Fig. 3 as a way to construct these molecules. The concave polygonal shape consisting of 20 equilateral triangles outlined by thick lines is cut out from the graphene plane. The polygon is then creased along the edges shared by the triangles and folded into a perfect icosahedron. The thus obtained shape is still not a fullerene since the details of its shape are wrong, but it has the same icosadeltahedral symmetry and the same connectivity and number of carbon atoms as the icosahedral fullerene does. The integers m and n that characterize the shape can now be interpreted as components of a two-dimensional vector \mathbf{A} in a basis of graphene unit cell vectors \mathbf{a}_1 and \mathbf{a}_2 denoted in Fig. 3,

$$\mathbf{A} = m\mathbf{a}_1 + n\mathbf{a}_2, \quad m, n > 0. \quad (7)$$

The \mathbf{A} vector is directed along the side of one of the twenty triangles making the icosahedron as illustrated in

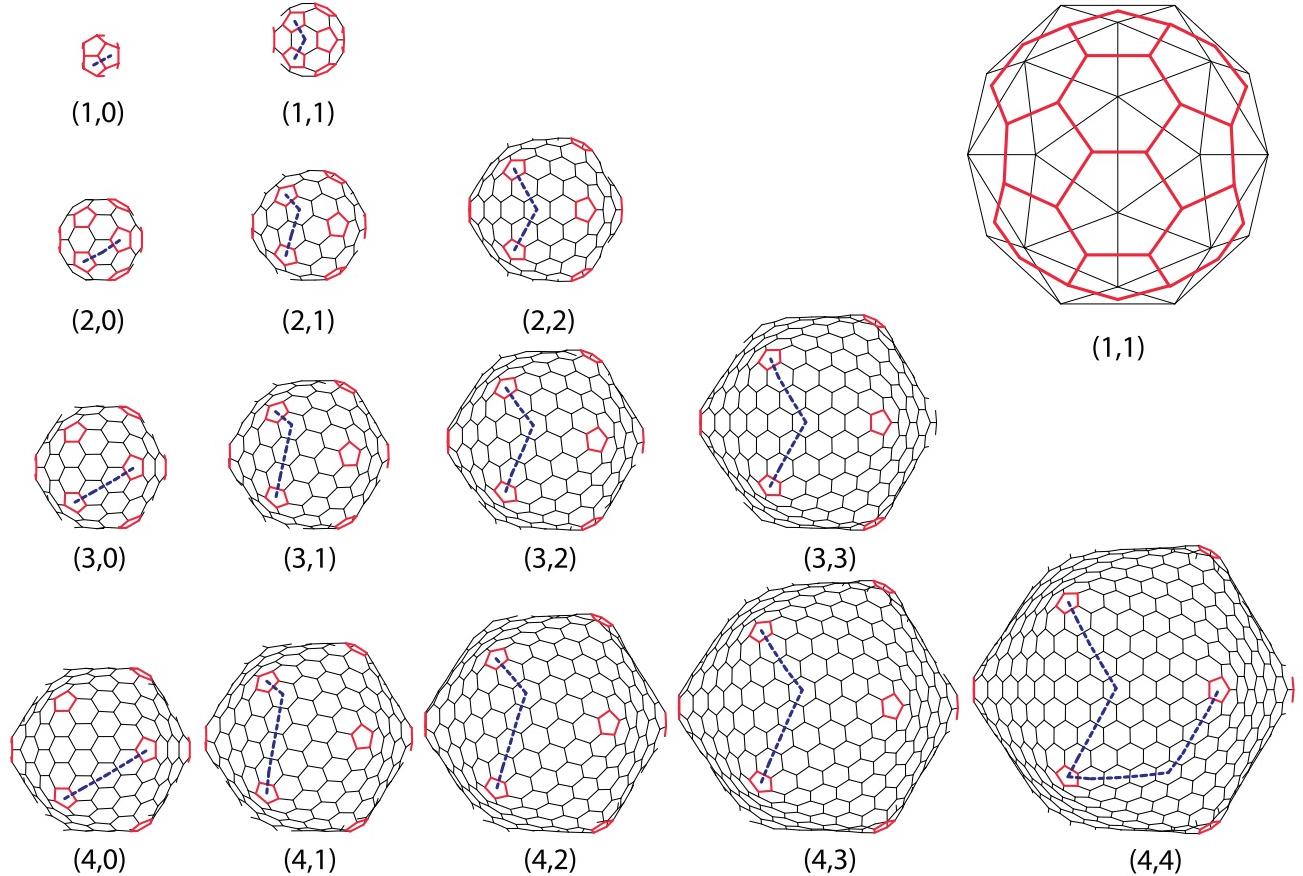


FIG. 2: Gallery of icosahedral fullerenes for $m > n$ and $m < 5$. For the sake of clearer representation the back sides of fullerenes are not shown. The carbon-carbon bond in all fullerenes is practically everywhere equal to 1.42 \AA , and this can be used to estimate their size. The upper-right corner of the figure contains comparison between (1,1) dome and (1,1) icosahedral fullerene (Buckminsterfullerene, not to scale with other depicted fullerenes). Note that these polyhedra are dual to each other.

Fig. 3. In this convention, the unit cell vectors \mathbf{a}_1 and \mathbf{a}_2 need to be chosen so that their vector product points from the paper towards the reader. This reproduces the jumping-to-the-left convention discussed in the previous section. The unfolding described here can also be applied to icosadeltahedra. The underlying lattice is triangular in that case. This procedure is very convenient for counting faces, edges and vertices and can be used to derive Eq. (1).

An important piece of information on fullerene molecules can be obtained from the Euler's theorem on polyhedra. Since exactly three bonds (or polyhedron edges) finish at each of the carbon atoms (polyhedron vertices) and the bond (edge) is shared by two atoms (vertices), it follows that

$$2e = 3v. \quad (8)$$

By definition, the fullerenes contain only pentagonal and hexagonal faces (carbon rings). Let us denote the number of pentagonal and hexagonal faces by f_5 and f_6 , respectively. The total number of faces is obviously given

by

$$f = f_5 + f_6. \quad (9)$$

Pentagonal and hexagonal faces are bounded by five and six vertices (atoms), respectively and each vertex (atom) belongs to exactly three faces. This means that

$$5f_5 + 6f_6 = 3v. \quad (10)$$

Combining these equations with Euler's theorem in Eq.(3) one obtains that

$$f_5 = 12. \quad (11)$$

This is obviously true for the icosahedral fullerenes discussed so far, but the equation holds for general fullerenes as long as they are topologically equivalent to a sphere (including e.g. C_{70}). In other words, every network of pentagonal and hexagonal ring of carbon atoms with spherical topology necessarily has five pentagonal rings. A relation between the number of carbon atoms in fullerenes and the number of hexagonal faces can also be obtained from the above consideration. It states that

$$v = 2(f_6 + 10). \quad (12)$$

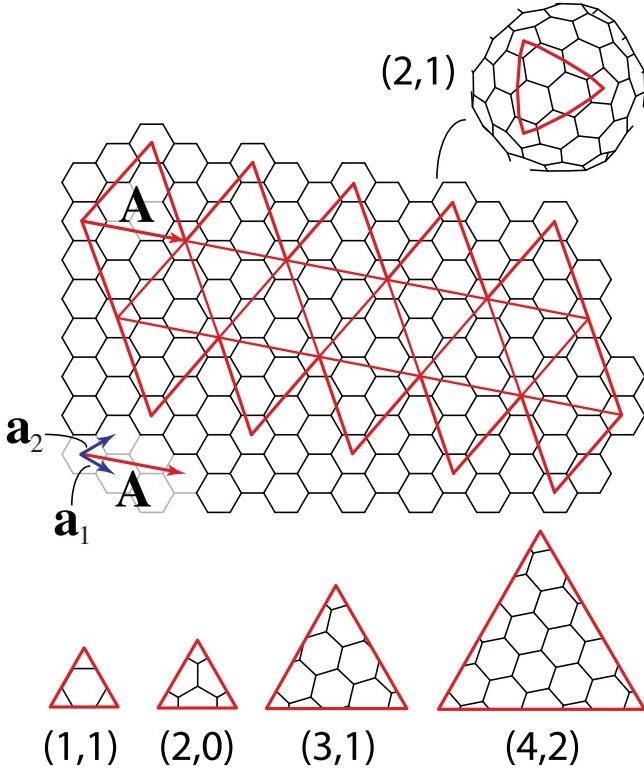


FIG. 3: Cut-and-fold construction of (2,1) icosahedral fullerene. The vectors \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{A} discussed in the text are denoted. The triangular faces of (1,1), (2,0), (3,1), and (4,2) fullerene-like icosahedra are shown in the bottom of the figure.

This means that the number of carbon atoms in the fullerene molecules is necessarily *even*. This, at first puzzling, piece of information was observed already in the mass spectra of carbon clusters obtained by laser vaporization from the graphitic sample¹⁵. Only signatures of clusters containing even number of carbon atoms were detected which can be nicely explained by assuming that the clusters detected were in fact fullerenes. Let us now specify the discussion of general fullerenes to the case of icosahedral fullerenes. Total number of carbon atoms in these molecules is

$$v = 20(m^2 + mn + n^2) = 20T, \quad (13)$$

and the number of carbon-carbon bonds is

$$e = 30T. \quad (14)$$

As shown earlier, there are exactly twelve pentagonal carbon rings and

$$f_6 = 10(T - 1) \quad (15)$$

hexagonal carbon rings.

Fullerenes with number of carbon atoms larger than about 120 were not clearly observed in the experiments described in Ref. 2. Thus, in addition to C_{60} , only

the C_{80} signature may in fact correspond to ($m = 2$, $n = 0$) icosahedral fullerene. Larger (giant) fullerenes can be observed in experiments but it is difficult to precisely determine their geometry and the spatial distribution of pentagonal carbon rings¹⁶. Carbon pentagons in graphitic samples have been observed using scanning tunneling microscopy¹⁷.

IV. CASPAR-KLUG CLASIFICATION OF VIRUSES: THE T-NUMBER

Viruses are particles made of DNA or RNA molecule (genome) protected by a coating made of proteins. Their size depends on the type of a virus⁷. The typical diameter of a virus is about 50 nm. For example the diameter of a herpes simplex virus is 125 nm, while polio virus is only 32 nm in diameter⁷. The information that is required to produce the proteins of the coating is contained in the viral RNA or DNA molecule. Once the virus penetrates the cell wall, the viral genome is delivered to the cell and the production of viral proteins starts. The proteins are produced by a cellular molecular machinery called ribosomes that can assemble proteins from amino acids by "reading" the information on the required sequence of amino acids that is coded in the viral RNA molecule. This process is called *translation* by biologists. A discussion of these marvelously complicated mechanisms would lead us far astray from the subject of interest. More information on virus "life" cycle can be found in Ref. 7 and on translation and transcription (a process for obtaining the information-carrying RNA from the DNA molecule) in textbooks on cell biology and chemistry (see e.g. Ref. 18).

In 1956 Crick and Watson¹⁹ proposed that the spherical protein coating (or capsid) probably has a platonic polyhedral symmetry i.e. that it is built of identical proteins assembled in a polyhedral shell. Caspar and Klug⁵ developed this notion further by noting that the quantity of information contained in the viral genome is quite small, so that only one or perhaps two to three different proteins can be produced from it. They considered different polyhedral shells made of identical proteins and deduced that icosadeltahedral ordering provides a structure in which all of the proteins are in surroundings that are to a best approximation equal of all the choices considered. They called this the principle of quasi-equivalence. The geometry behind the principle of quasi-equivalence is the one already discussed in the cases of icosadeltahedral geodesic domes and fullerenes.

In most of the "spherical" viruses, the proteins are grouped in clusters (capsomers) of five (pentamers) and six (hexamers). This is very often the case even if not all proteins are equal, i.e. when capsid consists of several types of proteins. In the assembled capsids, the twelve pentamers occupy the same spatial positions as carbon pentagons in fullerenes. The hexamers are equivalent to hexagonal carbon rings in fullerenes. Thus, viruses can

be constructed by connecting each of the vertices in pentagonal and hexagonal rings of the fullerenes with the ring centers and interpreting the thus obtained divisions of the pentagons and hexagons as the dividing lines between the viral proteins. In fact, the fullerene vertices need not be connected to the centers of the rings but to points lying on approximate normals to the pentagonal and hexagonal faces and passing through centers of the faces. This corresponds to capping the pentagons and hexagons with pentagonal and hexagonal pyramids, respectively, but the capping can also be performed in many other ways. The thus obtained polyhedron may be called omnincapped fullerene [all (*omni*) of the fullerene faces capped by pyramids or some other polyhedra]. This procedure is illustrated panels a) and b) of Fig. 4. The proteins are pieces of matter that have a certain equilibrium shape which is of course three-dimensional. Representation of protein capsomers by pyramids or any other polyhedron is thus approximate. Any three dimensional shape erected above the hexagon (pentagon) and having a six-fold (five-fold) symmetry with respect to rotations around the hexagon (pentagon) normal will serve as a representation of a viral hexamer (pentamer).

The classification of the symmetry of the capsid, however, does not depend on the shape of individual protein but only on the characteristics of the arrangement of all the proteins in the capsid (at least when all proteins are equal, see below). The symmetry of viruses is characterized in the same way as in the case of fullerenes: m and n integers are counted by "jumping" *through the centers of the capsomers* and using the convention of turning left after the first m jumps. If $m \geq n$, the virus is classified as a member of $T_{laevo} = m^2 + mn + n^2$ class (or simply T), and if otherwise, the virus is classified as a member of T_{dextro} (or T_d) class. The virus-like polyhedra depicted in panels a) and b) of Fig. 3 both have $T = 3$ symmetry, although the details of their shapes are quite different.

Total number of capsomers (c) in a T-class virus is obviously the same as the number points in the icosadeltahedral dome of T-symmetry,

$$c = 10T + 2. \quad (16)$$

Total number of proteins in a virus (p) is a sum of 60 proteins in 12 pentamers and $60(T-1)$ proteins in $10(T-1)$ hexamers. Alternatively (see Fig. 3) one can deduce that p for a virus of T-class should be the same as the number of faces in a dome of 3T-symmetry, i.e.

$$p = 60T, \quad (17)$$

so that both approaches give the same answer.

There may occur problems in identifying the symmetry of the capsid when several proteins form a capsid, or when building blocks of the capsid are not pentamers and hexamers but trimers (clusters of three proteins). The problem is illustrated by the shape in panel c) of Fig. 4. The building block of this shape is a protein trimer outlined by thick dashed lines. It consists of a darker

triangular protein (denoted by 1) and two brighter kite-shaped proteins (denoted by 2 and 3). This structure could be identified as belonging to $T = 1$ class, with only twelve "pentons" [outlined by thick full lines in Fig. 4c)] composed of five protein trimers (180 proteins in total). On the other hand, we could at least conceptually arrange the proteins in pentamers and hexamers as indicated by thick dash-dotted lines in Fig. 4c). In this case, hexamers would contain three pairs of 2- and 3-proteins from three trimers, while pentamers would consist of five 1-proteins from five different trimers. This would implicate that the shape belongs to $T = 3$ class of symmetry. Such viruses are called pseudo-T3 (or pT3) viruses. The problem with the identification could be resolved on physical grounds - if the binding energy between the proteins of the trimer is larger than between the proteins from different trimers, it makes sense to speak about the trimer as the basic building block and to identify the structure as belonging to $T = 1$ class. However, the problem in the mathematical sense occurs when there are two T numbers that can be divided without remainder (e.g. $T = 9$ and $T = 3$). In the most trivial case, every capsid with T-number T_1 could be interpreted as a $T = 1$ capsid consisting of T_1 -mers. In addition, every (m, m) capsid could in principle be thought of as $(m, 0)$ capsid made of trimers. The important question is again whether the conceptually obtained protein multimers make any sense as the strongly bonded elementary units.

Caspar and Klug quasi-equivalence principle predicts that there are only twelve pentameric capsomers, all other being hexameric. In year 1982 it became clear that there are viruses (e.g. SV-40 virus from polyomavirus genus) composed *only* of pentamers, but still retaining the icosadeltahedral symmetry of their arrangement²⁰. The concept of T-number is still valid in that case and the number of capsomers is still given by Eq. (16), but the total number of proteins is no longer given by Eq. (17). For such viruses, the total number of proteins is

$$p = 5c = 5(10T + 2). \quad (18)$$

Viruses, as fullerenes, should be considered as physical objects, i.e. their precise shape should be a result of interactions acting between proteins themselves and possibly between the proteins and viral DNA or RNA molecule. Shapes of viruses have recently been explored using a generic model of shells with icosadeltahedral symmetry^{21,22,23}. Application of physical methods to understand the energetics and assembly of viruses has been an area of very lively research in recent years (for a partial but quite readable glimpse of the field see Ref. 24).

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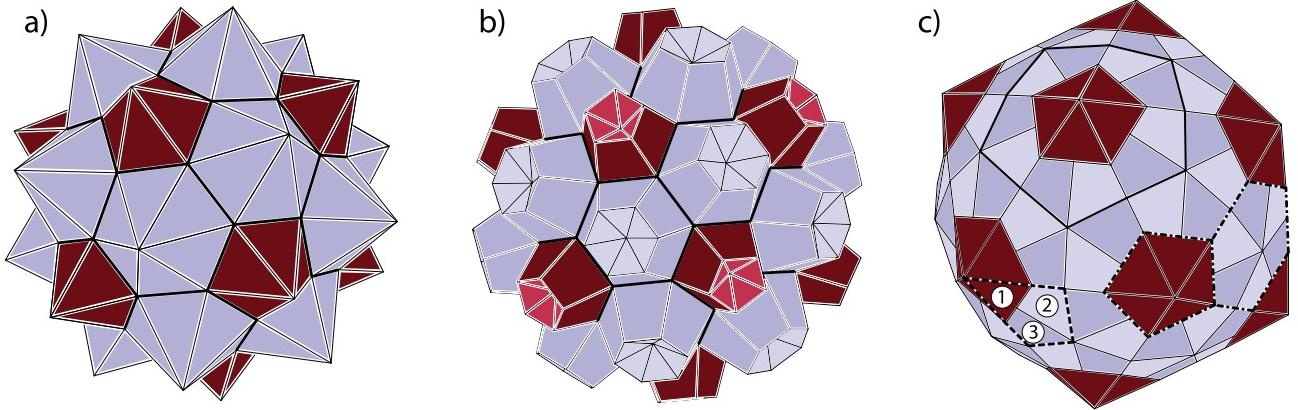


FIG. 4: Panels a) and b) represent polyhedral models of $T = 3$ viruses. These polyhedra can be termed as omnicapped truncated icosahedra or omnicapped Buckminsterfullerenes. The "pentamers" are colored in a darker tone and borders between "capsomers" are represented by thicker lines. The polyhedron in panel b) is quite similar to turnip yellow mosaic virus. Panel c) represents a model $T = 1$ (pT3) virus whose building block is a "protein trimer" outlined by dashed lines.

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